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THE FAMILY OF $\mathfrak{D}$-WEIGHTS FOR A TWO-ROOTED GRAPH

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Let $\Pi(G)$ be the set of paths of a particular class Π from the initial to the terminal root of a two-rooted (possibly directed) graph G. We consider the family of $\mathfrak{D}$-weights defined by

$$\mathfrak{D}(G)=\sum_{\Pi'\in\Pi_x(G)}(-1)^{|\Pi'|+1}$$

where $\Pi_x(G)$ is the family of subsets of $\Pi(G)$ which cover $x(G)$, the vertex set or the edge (arc) set of G.

A number of the common properties and interrelations of these weights are discussed. Some of the weights have been considered previously, [1, 2], in the context of percolation theory but here only combinatorial arguments are used.

1. Introduction

Certain of the $\mathfrak{D}$-weights defined in the abstract arise naturally in the context of percolation theory. They enter as the weights to be attached to the subgraphs in the calculation of the pair-connectedness of a graph, [1].

In the 'bond problem', where the edges E of a two-rooted graph G are open independently with probability p, the probability of a path of open edges from the initial to the terminal root is

$$P(p,G)=\sum_{E'\subseteq E} d(G_{E'})p^{|E'|}. \tag{1.1}$$

Here $G_{E'}$ is the graph induced by the subset of edges E' and the *weak d-weight* $d(G)$ is $\mathfrak{D}(G)$ with $x=E$ and $\Pi=S$, the set of self-avoiding paths from the initial root i to the terminal root j. The corresponding problem for directed graphs has also been considered [2]. In this case (1.1) is valid with E replaced by the arc set A and d replaced by the *directed weak d-weight* $\vec{d}(G)$, where $\vec{d}(G)$ is equal to $\mathfrak{D}(G)$ with $x=A$ and $\Pi=\vec{S}$, the set of self-avoiding paths which follow the directions of the arcs. The $\vec{d}$-weights are unique in that they take only the values ±1 or 0, [2].

The *strong D-weight* $D(G)$ is defined to be $\mathfrak{D}(G)$ with $x=V$ and $\Pi=S$. These weights arise in the site percolation problem where each vertex may be used as part of a path with probability p. The directed version of these weights, the

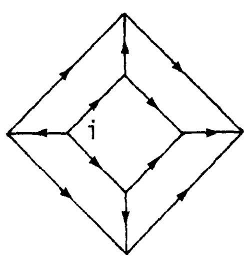
$\vec{D}$-weights, are considered here for the first time. It will be shown that the D and $\vec{D}$-weights may also be obtained by taking $x = V$ and $\Pi = N$, the neighbour-avoiding paths from i to j. These are paths n from i to j such that all edges of G which do not belong to a multi-edge and which have both vertices in $V(n)$ must belong to n.

Clearly $N \subseteq S$. In the directed case, for $n \in \vec{N}$ the arcs of G having both vertices in $V(n)$ are only required to be in n if they are directed parallel to n (an anti-parallel arc is one having its initial vertex occurring after its terminal vertex as the path is followed).

It has been shown [2] that if G is coverable by paths from i to j, then $\vec{d}(G) = 0$ if and only if G is cyclic. In any other case

$$\vec{d}(G) = (-1)^{t_{ij}+1} \tag{1.2}$$

where $t_{ij} = |E(G)| - |V(G)| + 2$, the maximal number of independent paths from i to j. It was hoped that the $\vec{D}$-weights would have maximum modulus unity, however

$\vec{D}$ (

j) = -2

The d-weights are of interest in pure graph theory since they depend only on the topology of the graph (vertices of degree two are irrelevant) and are related to the β-invariant of Crapo, [4]. Thus if G_d is the graph derived from G by including an extra edge connecting the roots and then treating the roots as ordinary vertices

$$\beta(G_d) = |d(G)|. \tag{1.3}$$

The graph G_d may of course be the derived graph of more than one G but the β invariant is an intrinsic property of the graph G_d having the same value for all two-rooted graphs G from which G_d may be derived.

Previous treatments [1, 2] of $\mathscr{D}$-weights have relied on probability arguments; here the development will use only combinatorial methods.

2. Alternative formulations of the $\mathscr{D}$-weights

The *path formulation* of the $\mathscr{D}$-weight given in the abstract is often less useful than the alternative we shall now develop.

Let H be a two-rooted graph with roots at i and j and let x be either its vertex or its edge set (arc set in the directed case). The subset x' of x generates a subgraph $G_{x'}$ of H which has elements x', together with its incident dual elements. [The vertices and edges (arcs) of a (directed) graph are said to be dual with respect to each other. An edge or arc is incident with a vertex set if both its vertices are contained therein].

Let $\Pi(x')$ be the set of paths of type Π from i to j on $G_{x'}$ (the paths must follow the orientation of the arcs in the directed case and when x refers to vertices $\Pi(x')$ is empty unless x' contains i and j). Define

$$\delta(x',\Pi)=\sum_{\Pi'\subseteq\Pi(x')}(-1)^{|\Pi'|} \tag{2.1}$$

so that

$$\delta(x',\Pi)=\begin{cases}1 & \text{if } \Pi(x')=\emptyset,\\ 0 & \text{if } \Pi(x')\neq\emptyset\end{cases} \tag{2.2}$$

and will therefore be known as the disconnectedness indicator.

2.1. Lemma. *If* (C1), *then the weight* $\mathfrak{D}(x',\Pi)$ *has the alternative form*

$$\begin{cases}\displaystyle\sum_{x''\subseteq x'}(-1)^{|x'\setminus x''|}\gamma(x'',\Pi), & \textit{for } x'\neq\emptyset,\\ \quad -1 & \textit{for } x'=\emptyset,\end{cases}$$

where $\gamma=1-\delta$ *is the connectedness indicator. The condition* (C1) *is*

$$C(x'',x',\Pi)=C(x'',x'',\Pi),\quad \textit{for } x''\subseteq x',$$

where

$$C(x'',x',\Pi)=\{\Pi'\subseteq\Pi(x')\mid x(\Pi')=x''\}. \tag{2.4}$$

Proof. We can express $\delta(x',\Pi)$ as a sum over subsets of x' and to this end we define

$$x(\Pi')=\bigcup_{p\in\Pi'}x(p)$$

where $x(p)$ is the set of elements of type x in the path p. Using (2.1) and (2.4)

$$\delta(x',\Pi)=\sum_{x''\subseteq x'}\;\sum_{\Pi'\in C(x'',x',\Pi)}(-1)^{|\Pi'|} \tag{2.5}$$

Now assuming C1 we obtain

$$\delta(x',\Pi)=\sum_{x''\in x'}\;\sum_{\Pi'\in C(x'',\Pi)}(-1)^{|\Pi'|} \tag{2.6}$$

with the relabelling $C(x'',\Pi)$ for $C(x'',x'',\Pi)$. Thus the second sum is now independent of x' and

$$\delta(x',\Pi)=-\sum_{x''\subseteq x'}\mathfrak{D}(x'',\Pi), \tag{2.7}$$

where

$$\mathfrak{D}(x'',\Pi)=\sum_{\Pi'\in C(x'',\Pi)}(-1)^{|\Pi|+1}.$$

Note $\mathfrak{D}(\emptyset,\Pi)=-1$.

Equation (2.7) may be transformed using Möbius inversion, [6], to yield the element formulation

$$\mathfrak{D}(x',\Pi) = -\sum_{x''\subseteq x'} (-1)^{|x'\setminus x''|}\delta(x'',\Pi) \tag{2.8}$$

The result now follows by substitution of δ by $1-\gamma$.

We now give a condition equivalent to C1 which is easier to check for the various cases which arise.

2.2. Lemma. *The condition* C2:

$$p\in\Pi(x'') \quad\Leftrightarrow\quad p\in\Pi(x') \quad \textit{and} \quad p\subseteq G_{x''} \quad \textit{for } x''\subseteq x',$$

is equivalent to C1.

Proof. This is straightforward and the details are omitted.

We now check C2 and hence C1 for the following special cases

A: $x=E$, $\Pi=N$,

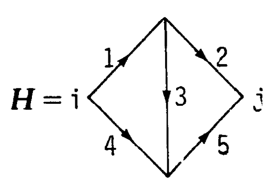
B: $x=V$, $\Pi=N$,

C: $x=E$, $\Pi=S$,

D: $x=V$, $\Pi=S$.

The corresponding directed cases will be denoted by $\vec{A}$ etc., and for these E represents the arc set and N and S are replaced by $\vec{N}$ and $\vec{S}$.

A and $\vec{A}$. C2 fails by considering



with $E'=\{1,2,3,4,5\}$ and $E''=\{1,3,5\}$, because $\{1,3,5\}\in\Pi(E'')$ and $\{1,3,5\}\notin\Pi(E')$. This counterexample is also good for the undirected case.

B and $\vec{B}$. C2 follows by construction of $G_{v'}$ and $G_{v''}$ since $V''\subseteq V'$ and all edges (arcs) in $G_{v''}$ are also in $G_{v'}$. For $\vec{B}$ replace N by $\vec{N}$.

In cases C and D, where $\Pi=S$, for any subgraph G'' of G' we have

$$p\in S(G'') \quad\Leftrightarrow\quad p\in S(G') \quad \text{and} \quad p\subseteq G'.$$

and C2 is a special case of this result.

3. The $\mathfrak{D}$-weights of a graph

In the previous section we defined the $\mathfrak{D}$-weight for a subset of the elements x of the graph H by (2.7) and showed that, subject to C1, (2.8) is an equivalent formula. It is clear from (2.8) that, given Π, $\mathfrak{D}(x', \Pi)$ depends only on the graph $G_{x'}$ generated by x' and not on the part of H which is outside $G_{x'}$. Also since

$$N(x'') \subseteq S(x'') \quad \text{and} \quad S(x'') \neq \emptyset \quad \Rightarrow \quad N(x'') \neq \emptyset,$$
$$\delta(x'', S) = \delta(x'', N) \quad \text{for } x'' \subseteq x' \tag{3.1}$$

with a similar result in the directed case; when considering only $\Pi = S$ or N we may therefore abbreviate to $\delta(x'')$. Thus subject to C1

$$\mathfrak{D}(x', S) = \mathfrak{D}(x', N). \tag{3.2}$$

For a two-rooted graph G, let $x(G)$ and $\Pi(G)$ be its elements of type x and its paths of type Π respectively and define

$$\Pi_x(G) = \{\Pi' \subseteq \Pi(G) \mid x(\Pi') = x(G)\} \tag{3.3}$$

We may then define its four different $\mathfrak{D}$-weights by

$$d(G) = \sum_{\Pi' \in S_E(G)} (-1)^{|\Pi'|+1} = -\sum_{E' \subseteq E(G)} (-1)^{|E(G) \setminus E'|} \delta(E') \tag{3.4}$$

$$D(G) = \sum_{\Pi' \in N_V(G)} (-1)^{|\Pi'|+1} = -\sum_{V' \subseteq V(G)} (-1)^{|V(G) \setminus V'|} \delta(V'). \tag{3.5}$$

The second form of each definition is valid since C1 holds for $x = E$, $\Pi = S$ and $x = V$, $\Pi = N$ respectively. By virtue of (3.2) and the fact that C1 holds for $x = V$, $\Pi = S$, we may also write

$$D(G) = \sum_{\Pi' \in S_V(G)} (-1)^{|\Pi'|+1}. \tag{3.6}$$

Similar formulae define $\vec{d}(G)$ and $\vec{D}(G)$ by replacing S by $\vec{S}$ etc. In referring to the four weights collectively we shall use $\mathfrak{D}(G)$ for which the general formulae are

$$\mathfrak{D}(G) = \sum_{\Pi' \in \Pi_x(G)} (-1)^{|\Pi'|+1} = -\sum_{x' \subseteq x(G)} (-1)^{|x(G) \setminus x'|} \delta(x'). \tag{3.7}$$

The weights $\vec{d}(G)$ and $\vec{D}(G)$ may be referred to collectively by $\vec{\mathfrak{D}}(G)$.

4. Rules relating $\mathfrak{D}$-weights

We derive rules by which the $\mathfrak{D}$-weight of a graph may be expressed in terms of the $\mathfrak{D}$-weights of smaller graphs. These rules are clearly useful in proofs by induction, as in [2], and also for computation. Here we assume that C1 is satisfied and restrict to $\Pi = S$ or N so that by (3.1) the argument Π may be dropped from $\mathfrak{D}(x, \Pi)$.

The proofs of the following three lemmas are left to the reader.

4.1. Lemma. (*The product rule for graphs with a cut vertex*). *Suppose the graph G has a cut vertex which divides it into two subgraphs G_1 and G_2; then*

$$\mathfrak{D}(G) = \mathfrak{D}(G_1) \cdot \mathfrak{D}(G_2). \tag{4.1}$$

4.2. Lemma. (*The product rule for parallel graphs*). *Suppose that the graph G may be divided into two subgraphs G_1 and G_2 such that any path between the roots i and j lies wholly within G_1 or G_2. Then for the weak $\mathfrak{D}$-weights,*

$$\mathfrak{D}(G) = -\mathfrak{D}(G_1) \cdot \mathfrak{D}(G_2). \tag{4.2}$$

4.3. Lemma. (*The loop rule.*) *The addition of a loop $[i, i]$ to a graph G leaves the strong $\mathfrak{D}$-weights unchanged, but makes the weak $\mathfrak{D}$-weights zero.*

It has been shown, [1, 2, 5], that the weak $\mathfrak{D}$-weights satisfy a rule $\mathfrak{D}(G) = \mathfrak{D}(G_\gamma) - \mathfrak{D}(G_\delta)$ where G_γ and G_δ are obtained from G by contracting and deleting any edge u ($\neq [i, j]$). For the directed case a further restriction was the requirement that the arc u must be incident out of i or into j.

We now obtain a similar result for strong $\mathfrak{D}$-weights by letting G_γ be the graph obtained by contracting an edge $[k, u]$ incident with u, (that is the edge $[k, u]$ is deleted, other edges $[l, u]$ incident with u are replaced by $[l, k]$ and u is deleted from the vertex set), and G_δ be the graph obtained by deleting vertex u.

4.4. Lemma. (*The deletion-contraction rule.*) *For any two-rooted graph G,*

$$\mathfrak{D}(x, \Pi) = \mathfrak{D}(x_\gamma, \Pi) - \mathfrak{D}(x_\delta, \Pi) \tag{4.4}$$

providing

$$\gamma(x') = \gamma(x'_\gamma), \quad \textit{for } x' \subseteq x, \tag{C3}$$

where $x'_\gamma = x'(G_\gamma)$.

Proof. From (2.3),

$$\mathfrak{D}(G) = \sum_{\substack{x' \subseteq x \\ u \in x'}} (-1)^{|x \setminus x'|}\gamma(x') + \sum_{\substack{x' \subseteq x \\ u \notin x'}} (-1)^{|x \setminus x'|}\gamma(x'). \tag{4.5}$$

Defining $x' = x'(G_\gamma)$ and $x'_\delta = x'(G_\delta)$ we see there is an obvious correspondence, by inclusion, between the subsets involved in the two sums of (4.5) and the subsets x'_γ, x'_δ of x_γ, x_δ respectively. Also it is clear that $\gamma(x') = \gamma(x'_\delta)$ when $u \notin x'$. Therefore by replacing $\gamma(x')$ by $\gamma(x'_\gamma)$ in the first summation of (4.5) the result follows.

Remark. It is easy to find examples of failure of C3 in the directed and undirected vertex case. We can combine the sufficient conditions for C3 to hold for all the various cases in the following result.

4.5. Lemma. *For a directed graph G, with $x = E$ or V, or an undirected graph with $x = V$, the condition C3 holds if the contracted edge e is adjacent to a root point and* *if in the directed case the edge is directed out of i or into j. If $x=E$ there are no restrictions on the choice of the edge e when G is undirected.*

Proof. For the case $x=E$ we observe that $\gamma(x')=1$ trivially implies that $\gamma(x'_\gamma)=1$. Conversely if $\gamma(x')=1$ then there is a path p_γ in x' and the natural inclusion $i:x'_\gamma \to x'$ of x'_γ in x' may induce a path $p=i(p_\gamma)$. If not then $p\cup\{e\}$ forms a path in x' in the undirected case (since the hypothesis of C3 ensures that $e\in x'$). If the graph is directed the conditions on e ensure that $i(p_\gamma)\cup\{e\}$ forms a directed path. It follows that $\gamma(x')=1$.

Now let $x=V$. The hypothesis of C3 ensures that the vertex $u\in x'$, and that $[k,u]$ is the edge to be contracted. The above constraints imply that k is a root point and that u is an adjacent vertex. Let $\gamma(x')=1$; then a path p in x' will exist which may or may not contain the vertex u. In the former case p clearly contracts to form a path on x'_γ if $[k,u]$ is an edge of p or the path composition of a loop at k together with a path on x'_γ. Clearly $\gamma(x'_\gamma)=1$. In the latter case $u\notin x(p)$ and so p is invariant under contraction and therefore p is a path on x'_γ. Thus we have shown that $\gamma(x')=1 \Rightarrow \gamma(x'_\gamma)=1$. Now suppose $\gamma(x'_\gamma)=1$; then there is a path p_γ on x'_γ. Consider its inclusion $i(p_\gamma)$ in x' which may be a (directed) path in x'. If not, then the terminal vertices are u and a root point ($\neq k$). Clearly we can now construct a path by adding $[k,u]$ to $i(p_\gamma)$. Moreover the orientation of $[k,u]$ is defined so that a path exists in the directed case.

The condition C3 holds in a more general situation when $x=E$. This property is needed to prove the edge-replacement rule, (see below). Consider a two-rooted graph G, which has a subgraph G_0 with two-point contact in G at the roots of G_0. Let $x(G)=x$ and $x(G_0)=x_0$. Then C3 holds for x if we carry out contractions and deletions on x_0 at its root points in the usual way. So we may assume that x'_γ is obtained from x', $x'\subseteq x$, by contraction of an edge e of G_0 where the contraction of edge e in G_0 satisfies C3. Before considering the edge-replacement rule we need the following lemma.

4.6. Lemma. (*The multi-edge rule.*) *Let G^+ be a graph constructed from G by adding an edge (arc) a which is parallel, with the same orientation in the directed case, to an edge (arc) of G thereby forming a multi-edge (arc). Then the strong-weights are equal for G and G^+ and the weak-weights differ only in sign.*

Proof. The arguments for D and $\vec{D}$ follow straight from the definitions in Section 3. For the weak-weights $E^+\equiv E(G^+)=E\cup a$, and so by (2.3)

$$\begin{aligned} d(G^+) &= \sum_{E'\subseteq E} \gamma_+(E')(-1)^{|E'\setminus E|} + \sum_{E'\subseteq E} \gamma_+(E'\cup a)(-1)^{|E\setminus E'|} \\ &= -\sum_{E'\subseteq E} \gamma(E')(-1)^{|E\setminus E'|} + \sum_{E'\subseteq E-a} \gamma_+(E'\cup a)(-1)^{|E\setminus E'|} \\ &\quad +\gamma(E'\cup a\cup \bar{a})(-1)^{|E\setminus(E'\cup \bar{a})|} \end{aligned} \tag{4.6}$$

Where $\bar{a}$ is the edge parallel to a. Now $\gamma_+(E' \cup a \cup \bar{a}) = \gamma_+(E' \cup a)$ so that the second summation is zero and therefore $d(G') = -d(G)$. The same arguments holds for $\vec{d}$.

We can now obtain the result:

4.7. Lemma. (*The edge-replacement rule.*) *If an edge (arc) $[i_0, j_0]$ of the graph H is replaced by a two-rooted graph G_0, (the roots being identified with i_0 and j_0), with at least one edge, then the resulting graph G has weak-weights given by*

$$\mathscr{D}(G) = \mathscr{D}(H) \cdot \mathscr{D}(G_0) \tag{4.7}$$

Proof. The graph G_0 has two-point contact in G and we may assume that the edges E_0 of G_0 are $\Pi(G)$-coverable since otherwise $\mathscr{D}(G_0) = \mathscr{D}(G) = 0$ and the result follows trivially. Also the trivial situation of G_0 being a parallel graph may be excluded. Therefore we can apply the deletion-contraction rule to an edge u of G_0 incident with i_0 which is not $[i_0, j_0]$. Thus $\mathscr{D}(G) = \mathscr{D}(G_\gamma) - \mathscr{D}(G_\delta)$ and assuming (4.7) holds for G_γ and G_δ we have

$$\mathscr{D}(G) = \mathscr{D}(H) \cdot (\mathscr{D}(G_{0_\gamma}) - \mathscr{D}(G_{0_\delta}))$$

by using Lemma 4.4 and hence (4.7) is true for G. But G_{0_γ} and G_{0_δ} also have two-point contact in G and so the argument may be repeated. This reduction process will result in the inserted graph becoming a multi-edge to which we can apply Lemma 4.6.

Remark. The result fails for D-weights since a further reduction is possible. For example, suppose that at some stage a graph arises such that G_0 is the 2-chain $[i_0, l, j_0]$, then deletion of the vertex l leads to a graph for which (4.7) does not hold true.

There are also relations between $\mathscr{D}$-weights of different types. The weak-strong relations are:

$$D(G) = \sum_{E' \in \mathscr{E}(V)} d(G'), \qquad \vec{D}(G) = \sum_{E' \in \mathscr{E}(V)} \vec{d}(G') \tag{4.8}$$

where $\mathscr{E}(V)$ is the set of all subsets of E having incident vertexset V. There is also a weak-weight directed-undirected relation, [2],

$$d(G) = \sum_{H \in \partial(G)} \vec{d}(H)$$

where $\partial(G)$ is the set of all directings of G.

5. Percolation theory

Consider the two-rooted graph G and suppose that each element $u \in x$ has probability $1 - p_u$ of being deleted independently of all other elements. The probability that there is no path of type Π form i to j is

$$Q_{ij}(G)=\sum_{x'\subseteq x(G)}\delta(x',\Pi)\prod_{u\in x'}p_u\prod_{v\in \bar{x}'}(1-p_v)$$

where $\bar{x}'=x(G)\backslash x'$. Expanding the second product

$$\begin{aligned}Q_{ij}(G)&=\sum_{x'\subseteq x(G)}\delta(x',\Pi)\sum_{x''\supseteq x'}(-1)^{|x''\backslash x'|}\prod_{u\in x''}p_u\\&=\sum_{x''\subseteq x(G)}\prod_{u\in x''}p_u\sum_{x'\subseteq x''}(-1)^{|x''\backslash x'|}\delta(x',\Pi)\\&=-\sum_{x''\subseteq x(G)}\mathcal{D}(x'',\Pi)\prod_{u\in x''}p_u\end{aligned}$$

where we have used (2.11) and the empty product corresponding to $x''=\emptyset$ has the value unity. The pair connectedness [1] $P_{ij}=1-Q_{ij}$ is given by

$$P_{ij}(G)=\sum_{\emptyset\neq x''\subseteq x(G)}\mathcal{D}(x'',\Pi)\prod_{u\in x''}p_u.$$

where we have used $\mathcal{D}(\emptyset,\Pi)=-1$.

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